High-energy scale revival and giant kink in the dispersion of a cuprate superconductor

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(Dated: February 5, 2008)

In the present photoemission study of a cuprate superconductor $Bi_{1.74}Pb_{0.38}Sr_{1.88}CuO_{6+\delta}$, we discovered a large scale dispersion of the lowest band, which unexpectedly follows the band structure calculation very well. The incoherent nature of the spectra suggests that the hopping-dominated dispersion occurs possibly with the assistance of local spin correlations. A giant kink in the dispersion is observed, and the complete self-energy containing all interaction information is extracted for a doped cuprate in the low energy region. These results recovered significant missing pieces in our current understanding of the electronic structure of cuprates.

The interplay between different energy scales of a physical system usually holds the keys of its various fascinating properties. For cuprate superconductors and their parent Mott-insulator, the bandwidth of the so-called Zhang-Rice singlet band [1] has been intriguingly illustrated in numerical studies and experiments[2, 3, 4, 5, 6] to be $2.2J$ instead of $4t$, J being the magnetic exchange interaction, and t being the hopping integral. This renormalization of the effective bandwidth from $4t$ to $2.2J$ in cuprates was considered to be an important step toward the ultimate understanding of the high temperature superconductivity[7], which highlights the importance of magnetism. In practice, such effective band has been widely adopted in various self-energy analysis of the low energy kinks in the cuprate dispersion in terms of either electron-phonon[8, 9, 10] or electron-magnon[11, 12] interactions.

However, the above effective bandwidth largely depends on an extrapolation in doped cuprate, since the quasiparticle dispersion in a large region near the Brillouin zone center, Γ, has not been identified so far, possibly due to very broad lineshape. Based on an effective tight binding model [13], hopping parameters could be fitted out of the partial quasiparticle dispersion observed in the vicinity of the Fermi surface up to 0.35 eV below the Fermi energy E_F. The bandwidth of the occupied part is then extrapolated to be about 0.4 eV.[13, 14] Recent technological advances enable us to study electronic structure in a much wider momentum window. It is therefore pertinent to reexamine the "missing dispersion" near Γ, and check whether this extrapolation is justified. In this paper, we report the discovery of such missing dispersion in the photoemission data of a cuprate superconductor $Bi_{1.74}Pb_{0.38}Sr_{1.88}CuO_{6+\delta}$ (Bi2201). We found that sections of coherent and incoherent spectra piece together a full dispersion actually on the order of $4t$ *again*. This large scale dispersion unexpectedly follows the band structure calculation very well, except that there is a giant kink at low energies. These findings provide a fresh picture on the subtle interplay of different energy scales in cuprates. Moreover, the experimental bare band was retrieved from the data, which enables the experimental retraction of the full self-energy of a doped cuprate. So far, only partial self-energy has been studied in most previous experiments. Therefore, the revelation of such a critical quantity that contains the complete interaction information would provide really strong constraints on theory.

Highly overdoped $Bi_{1.74}Pb_{0.38}Sr_{1.88}CuO_{6+\delta}$ single crystal was prepared by floating-zone technique and subsequent annealing. The superconducting phase transition temperature T_c is 5K, indicating the hole concentration is very close to the superconductor/metal phase boundary. ARPES experiments were performed at the Beamline 9 of Hiroshima Synchrotron Radiation Center (HiSOR), which is equipped with a Scienta R4000 electron analyzer. The angular resolution is 0.3° and the energy resolution is 10 meV. The data were taken at 20 K with 22.5 eV photons in the wide angle mode, which covers more than 30°. This enables the identification of broad features in momentum distribution curves, which is crucial for the observation made here. The samples were aligned by Laue diffraction, and cleaved in-situ in ultra-high vacuum better than $5 \times 10^{-11}\, mbar$.

ARPES intensity map for a highly overdoped Bi2201 in a wide energy and momentum range is shown in Fig. 1a along the $(0,0) - (\pi,\pi)$ or nodal direction. Guided by the thick lines, one can clearly observe two hybridized bands. The low energy one would have dispersed down to ~ 1.6 eV below E_F (*i.e.,* $4t$, *instead of* $2.2J$), if it had not intersected the high energy band around -1.2 eV. Because the broad MDC feature is still much narrower than the wide angular window of the newly developed analyzer, artifacts such as the inhomogeneity across the two dimensional detector can be excluded. The dispersion within [-0.9 eV, -0.4 eV] is clearly visible in the mo-

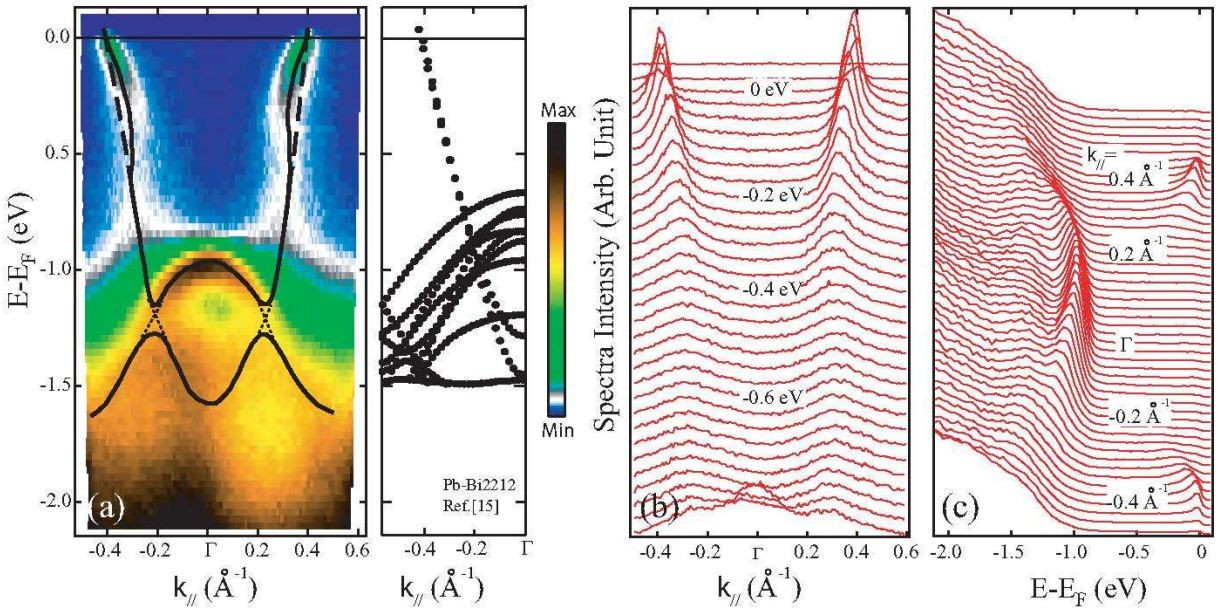

FIG. 1: Large energy scale dispersion of Bi2201. (a), Photoemission intensity as a function of energy and momentum along the nodal direction. The thick lines indicate the experimentally measured dispersion. The thick dashed lines indicate the linear behavior of the bare band as predicted by LDA calculations. The slight asymmetry of the data are due to matrix element effects and possible small misalignment from the nodal direction. The right side shows the LDA band structure calculated up to 1.5 eV for the nodal direction of Bi2212 from Ref.[15]. (b), Selected momentum distribution curves, and (c), Energy distribution curves of data plotted in panel (a).

mentum distribution curves (MDC's) (Fig.1b). The dispersion and smooth connection to the strong feature near Γ confirm that it is not caused by some secondary electron background. Therefore, the strong feature around Γ is part of the same band as the quasi-particle band near E_F. On the other hand, their relation is unobvious in the energy distribution curves (EDC's) in Fig.1c, where the dispersion within [-0.9 eV, -0.4 eV] cannot be resolved. The band and dispersion energy scales identified in Fig. 1a agree with the recent local density functional (LDA) band structure calculation of Pb-doped bilayer $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) compound very well (right side of Fig. 1a)[15], as the bilayer splitting is minimal along the nodal direction[16]. The strong feature near Γ is shown mostly consisted of other Cu d and O p orbitals than those for the band close to E_F. The well preserved quasiparticles at such high energies (Fig. 1c) indicate correlation effects are quite weak for these orbitals. The interesting difference is that the experimental dispersion near E_F deviates from the straight line in the band calculation, and exhibits a large kink.

This wide dispersion exists over a large region of the Brillouin zone. As shown in Fig.2, besides the nodal cut in Fig. 2a, it is also observed in cut #2 and #3, which is half way between the nodal and antinodal regions. In cut #4 and #5, the renormalized band is located near E_F. A weak feature also exists at high energy, although there is no missing band dispersion. However, compared with cut #1-3, the high energy feature in cut #4-5 is weaker, and extends straight into high energies, does not show a connection with the high energy band. On the other hand, the broad lineshape and the resemblance do suggest the high energy features observed in cut #1-3 contain significant incoherent weight. Recently, high energy dispersion beyond the $2.2J$ and incoherent lineshape in the Mott insulator $Ca_2CuO_2Cl_2$ were reported [17], which have also been observed in various numerical studies of hole motion in an antiferromagnetic spin background[4, 18, 19]. The hole concentration of the heavily overdoped system under study is about 1/4, so that long range antiferromagnetic order no longer exists, and even long range spin fluctuations diminish[20]. However, the neighboring sites of a hole mostly are still occupied by spins, and the short range spin correlations are still strong, even though the quasiparticle peak near E_F is very well defined[14, 21]. Consistently, the MDC widths at high binding energies are around 0.2 $Å^{-1}$, which correspond a short length scale of 5 Å. It has been shown that a hole dressed with heavy local spin-flip cloud would enhance the electron-phonon interaction greatly[22]. In the strong electron-phonon coupling regime, the spectrum could be shown to be dominated by the incoherent part due to multiple phonon excitations, and yet follows the bare band structure dispersion, while the quasipar-

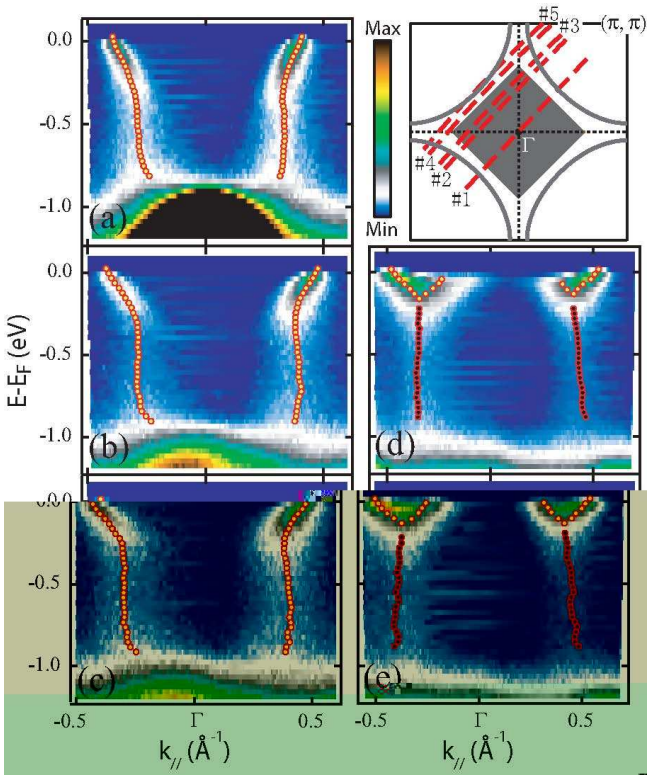

FIG. 2: Momentum dependence of the high energy dispersion. (a-e) Photoemission intensity taken along the cut #1-5 respectively in the Brillouin zone as illustrated in the inset on the top right corner, where large energy scale dispersion happens in the dark region. The yellow dots mark the position of the measured band dispersion, while the black dots in (d) and (e) indicate the centroid of the incoherent feature.

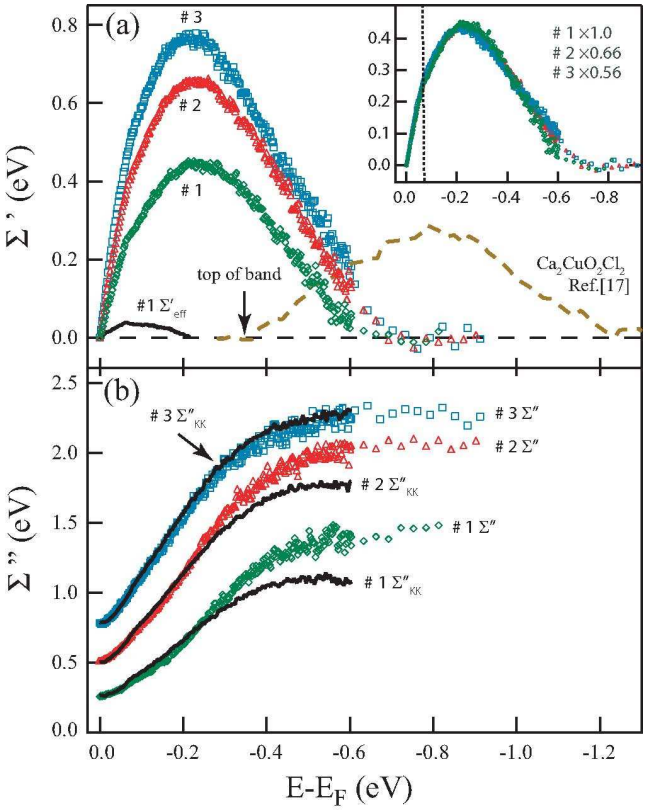

FIG. 3: Full self-energy of the Bi2201 extracted from the measured dispersion. (a) the real part of the self energy for cut #1 (diamonds), #2 (triangles), and #3 (squares). The solid line is real part of the self energy for the conventional low energy kink, Σ'_{eff}. The dashed line is the high energy kink observed in parent Mott insulator compound $Ca_2CuO_2Cl_2$ for comparison purpose[17], the arrow marks the top of its band. Inset: The Σ' for cut #1-3 could be re-scaled to match each other, where the dashed line indicates the low energy kink position. (b) Imaginary part of the full self-energy as a function binding energy. The data were shifted up by 0.25 eV and 0.5 eV for cut#2 and #3 respectively. The solid curves are the imaginary part calculated from the real part of the self-energy based on Kramers-Kronig transformation.

ticles are renormalized to the vicinity of E_F with little weight[23, 24]. Lately, the broad lineshape in the undoped La_2CuO_4 has been well simulated when strong electron-phonon interactions were considered[25]. Therefore, the observed bare band dispersion of the incoherent spectral weight in doped cuprates could possibly be attributed to strong electron-phonon interactions enhanced by local spin flip cloud around the hole [14, 22]. While for the quasiparticles near -1 eV, as these high energy orbitals are less affected by the spin-flip cloud at the low energy orbitals, the hole can travel more freely. Consequently, an anomalous electronic structure for Bi2201 is revealed: well defined coherent quasiparticles exist at both high energies and low energies, giving a total occupied band width of 1.2 eV, while incoherent features that follow the bare band dispersion dominate the intermediate energy region. This anomalous dispersion covers most of the Brillouin zone as shown by the dark region in the inset of Fig.2.

One remarkable observation in Figs. 1 and 2 is the giant kink structure in the dispersion compared to the band structure calculation. The large scale dispersion observed here and the linear dispersion behavior near E_F predicted by LDA calculations provide a rare chance to extract the full self-energy, Σ, of a strongly correlated system, which reflect all correlation effects in the system. Fig. 3a shows the real part of the self-energy, Σ' which is the difference between the bare band (*e.g.* the dashed line in Fig. 1a) and the measured band. Σ' contains contributions from all interactions. In previous studies, because of the lack of bare band information, a fraction of the self energy, Σ'_{eff} was retrieved by assuming a local effective band structure[26]. The resulting partial self-energy was argued to contain information on interactions between electrons and certain bosons. As shown in Fig. 3a, Σ'_{eff} is only a small fraction of Σ'. Away from the nodal cut, Σ' increases toward the antinodal direction. Interestingly, as shown in the inset of Fig.

3a, $\Sigma^{'}$ of different cuts can be scaled to a universal curve, where even the details of the low energy kink structures matches each other. These raise the questions whether the low energy kink is just a part of a large scale electronic effects, and whether the kink extracted in conventional analysis cleanly represents the interaction between electrons and bosons[8, 9, 10, 11, 12]. The $\Sigma^{'}$ extracted from the high energy dispersion data of $Ca_2CuO_2Cl_2$ is also plotted in Fig.3a for comparison[17]. The qualitative resemblance between a Mott insulator and a highly overdoped cuprate here remarkably illustrates their similar short range behavior. On the other hand, the observed doping dependency also provides additional evidences for further refinement of the role that spins and lattice play in the large energy scale dispersion.

The imaginary part of the self-energy $\Sigma^{''}$ is shown in Fig. 3b, which is the product of the MDC width and the bare band velocity (the slope of the dashed line in Fig. 1a). Generally, it increases rapidly in the first 0.35 eV, then gradually saturates at high binding energies, indicating that the spectrum is dominated by incoherent excitations here. For comparison, $\Sigma^{''}_{KK}$, the Kramers-Kronig transformation of $\Sigma^{'}$, is shown here.[27] The good agreement between $\Sigma^{''}$ and $\Sigma^{''}_{KK}$ on the low energy side for all three cuts confirms that the full self-energy has been reliably extracted at least in the first 300 meV below E_F. On the other hand, the deviation at high energies again reflects the incoherent nature of the electronic structure there. We note that the large amplitude and energy expansion of Σ at such high doping is quite anomalous. The self energy measured here provide direct and critical information for the development of theory for cuprates.

To summarize, we have presented a global picture of the electronic structure and the interplay of t and J in a highly overdoped cuprate. Contrary to previous perceptions, the band width is still determined by t, although the low energy quasiparticles exist in the J energy scale. On the other hand, the high energy dispersion over a large fraction of the Brillouin zone may still be attributed to J through the polaronic effects induced by strong local spin correlations. Moreover, various intriguing new information is revealed under this global picture, such as the much larger amplitude and energy expansion of the giant kink compared with the low energy kink discussed before, the universal scaling of $\Sigma^{'}$, and resemblance to the insulator. Since the high energy and local physics set the footing for low energy properties, these findings provide a comprehensive view of the different energy scales in the problem. More over, the full self-energy extracted for the the low energy (<300 meV) put strong quantitative constraints on models that are designed to understand high temperature superconductivity in a realistic cuprate material.

D.L.F. would like to thank Profs. Z. Y. Weng, and J. P. Hu for helpful discussions. This work was supported by NSFC and MOST (973 project No:2006CB601002) of China, Science & Technology committee of Shanghai, and the Core-University Program of JSPS.

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